The response to dynamical modulation of the optical lattice for fermions in the Hubbard model

Zhaoxin Xu[1], Simone Chiesa[2,3], Shuxiang Yang[1], Shi-Quan Su[1], Daniel E. Sheehy[1], Juana Moreno[1], Richard T. Scalettar[2], and Mark Jarrell[1]
[1]*Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA*
[2]*Physics Department, University of California, Davis, CA 95616, USA*
[3]*Physics Department, University of Tennessee, Knoxville, TN 37996, USA*
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Fermionic atoms in a periodic optical lattice provide a realization of the single-band Hubbard model. Using Quantum Monte Carlo simulations along with the Maximum Entropy Method, we evaluate the effect of a time-dependent perturbative modulation of the optical lattice amplitude on atomic correlations, revealed in the fraction of doubly-occupied sites. Our treatment extends previous approaches which neglected the time dependence of the on-site interaction, and shows that this term changes the results in a quantitatively significant way. The effect of modulation depends strongly on the filling– the response of the double occupation is significantly different in the half-filled Mott insulator from the doped Fermi liquid region.

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A number of key properties of strongly correlated electron systems appear to be well described by simplified tight-binding Hamiltonians. For example, the square lattice Hubbard model, with one particle per site, is known to possess the long range antiferromagnetic order manifest in the parent compounds of high temperature superconductors, whose CuO_2 sheets have square arrays of copper atoms with one hole per $3d$ shell. There are many analytic and numerical clues that suggest the doped Hubbard model might also possess the d-wave superconducting phase exhibited by the cuprates, as well as other nontrivial properties including stripes and pseudogap physics [1]. If this could be demonstrated rigorously, it would provide important insight into the mechanism of superconductivity in these materials.

Ultracold atomic systems offer an opportunity for closer connection between experiments and calculations for such model Hamiltonians. At present, experiments on fermionic atoms are exploring temperatures T which are of the order of the hopping integral J_0, probing correlations such as double occupancy, D, and short range spin order that develops at that temperature scale. In particular, the evolution of D with the ratio of interaction strength U to hopping J_0 has been shown to indicate the presence of a Mott metal-insulator transition [2, 3]. The presence of a Mott gap in the excitation spectrum has also been inferred through peaks in D which arise through a dynamic modulation of the optical lattice depth V [2].

The possibility that such a modulation might provide a useful probe was first suggested by Kollath *et al.* [4], based on earlier work with bosonic systems [5]. Using a time dependent Density Matrix Renormalization Group method, it was shown that a peak existed in the induced double occupation at a frequency ω which matched the interaction strength U. In this treatment, the response kernel was approximated to include only changes δJ in the hopping operator, neglecting corresponding variation δU in the on-site interactions. Within this approximation, the authors emphasized that the measurement was sensitive to near neighbor spin correlations, and the exchange gap, as well as the charge gap.

This 'modulation spectroscopy' has been further explored theoretically by Huber[6] and Sensarma[7]. In the former work, the frequency dependence of the shift in D was studied in the atomic and two particle limits, and within a slave boson mean field theory. The latter work focused on observing local antiferromagnetic order at the superexchange scale. As with the earlier study of Kollath, in both of these papers, the modulation was assumed to couple only to the kinetic energy.

In this paper, we extend previous work by studying the effect of both the modulation of the tunneling strength δJ and of the on-site interaction strength δU due to varying the optical lattice depth V, for the two dimensional repulsive fermionic Hubbard Hamiltonian. The modulation by δU is shown to be quite significant in the parameter range of interest to current experiments. We find that the filling of the system plays a very important role in the response. Crucially, through the use of Determinant Quantum Monte Carlo (DQMC) [8] and the maximum entropy method [9, 10], we provide results which treat the electron-electron correlations exactly.

In the low energy limit, two species of repulsively interacting fermions confined to a periodic optical potential with wavelength λ and amplitude $V(t)$ can be described by the one-band Hubbard model [11],

$$\hat{H} = -J\hat{K} + U\hat{D} - \mu\hat{N}, \tag{1}$$

where the hopping or kinetic-energy operator is $\hat{K} = \sum_{<ij>,\sigma}[\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}]$, $\hat{D} = \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the double occupancy, and $\hat{N} = \sum_i \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, the total number of par-

ticles, with $\hat{c}^{\dagger}_{i\sigma}(\hat{c}_{i\sigma})$ the fermion creation (annihilation) operator, $\sigma =\uparrow,\downarrow$ the spin index, $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}$, and μ the chemical potential. The hopping (J) and interaction (U) can be expressed as [11] $J \approx (4/\sqrt{\pi})\, E_R\, v^{3/4} \exp(-2\sqrt{v})$ and $U \approx 4\sqrt{2\pi}\,(a_s/\lambda)\, E_R\, v^{3/4}$, where $v = V/E_R$ is the ratio of lattice depth to recoil energy, and a_s is the short ranged s-wave scattering length.

It is clear from these expressions that a small time-dependent modulation of V changes both J and U. Writing $V(t) = V_0 + \delta V \sin(\omega t)$ and expanding J and U in the limit $\delta V \ll V_0$ yields $\hat{H} = \hat{H}_0 + \delta\hat{H}\sin(\omega t)$ with $\hat{H}_0$ given by Eq. (1) with J replaced by J_0 and U by U_0, and $\delta\hat{H} = -\delta J\hat{K} + \delta U\hat{D}$ with the time-dependent perturbations

$$\begin{aligned}\delta J &= J_0\Big(\frac{3}{4} - \sqrt{\frac{V_0}{E_R}}\Big)\frac{\delta V}{V_0},\\ \delta U &= \frac{3}{4}U_0\frac{\delta V}{V_0}.\end{aligned}\tag{2}$$

For $\delta V > 0$, we have $\delta J < 0$ and $\delta U > 0$ so that an increase in the optical lattice amplitude suppresses hopping and increases the Hubbard repulsion. We emphasize that one cannot a priori neglect δJ or δU as they can be of the same order of magnitude if using the experimental parameters as in Ref. 2.

Our aim is to understand how such a simultaneous modulation of the hopping and interaction parameters, as provided by fermions in a time-dependent optical lattice, probes fermion correlations in the Hubbard model. To this end, we study the time dependence of the average double occupancy $D(t) = \langle\hat{D}\rangle$. Within standard time-dependent perturbation theory, $D(t)$ satisfies, to linear order,

$$D(t) = D(t_0) - i\int_{t_0}^{t} dt'\, \langle[\hat{D}(t), \delta\hat{H}(t')]\rangle_0 \sin\omega t',\tag{3}$$

where $\langle\hat{\mathcal{O}}\rangle_0 = Z_0^{-1}\mathrm{Tr}e^{-\beta\hat{H}_0}\hat{\mathcal{O}}$ and $\hat{\mathcal{O}}(t) = \mathrm{e}^{i\hat{H}_0 t}\hat{\mathcal{O}}\mathrm{e}^{-i\hat{H}_0 t}$. Equation (3) can be simplified by rewriting $\delta\hat{H}$ in terms of $\hat{H}_0$ as $\delta\hat{H} = (\delta J/J_0)\,(\hat{H}_0 + U_0[\alpha-1]\hat{D})$, with $\alpha = \left(1 - \frac{4}{3}\sqrt{\frac{V_0}{E_R}}\right)^{-1}$. When inserted into Eq. (3), the first term will give a vanishing contribution, leading to

$$D(t) = D(t_0) + \frac{U_0}{J_0}(\alpha-1)\int_{t_0}^{\infty} dt'\, \delta J\chi_{\mathrm{DD}}(t-t')\sin\omega t',\tag{4}$$

where $\chi_{\mathcal{O}\mathcal{O}}(t-t') = -i\langle[\hat{\mathcal{O}}(t), \hat{\mathcal{O}}(t')]\rangle_0\,\theta(t-t')$. Formally setting $\alpha = 0$ amounts to neglecting the modulation of the interaction term. In contrast, experimentally, α typically varies within the range $-0.41 < \alpha < -0.28$. The simplification leading to Eq. (4), can be generalized to show that $\chi_{\mathrm{DD}}(t) = \big(J_0/U_0)^2\chi_{\mathrm{KK}}(t)$, a fact that we shall use below in our analysis.

Numerically, we calculate the imaginary-time quantity $\chi_{\mathrm{DD}}(\tau)$ from Determinant Quantum Monte Carlo simulations [8] and analytically extrapolate to the corresponding imaginary part of the real frequency quantity $\chi''_{\mathrm{DD}}(\omega)$ by inverting

$$\chi_{\mathrm{DD}}(i\nu_n) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, \frac{\chi''_{\mathrm{DD}}(\omega)}{i\nu_n - \omega},\tag{5}$$

via the Maximum Entropy method [9, 10]. In Eq. 5 $i\nu_n = 2n\pi T$ is the bosonic Matsubara frequency, T is the temperature, and ω the real frequency.

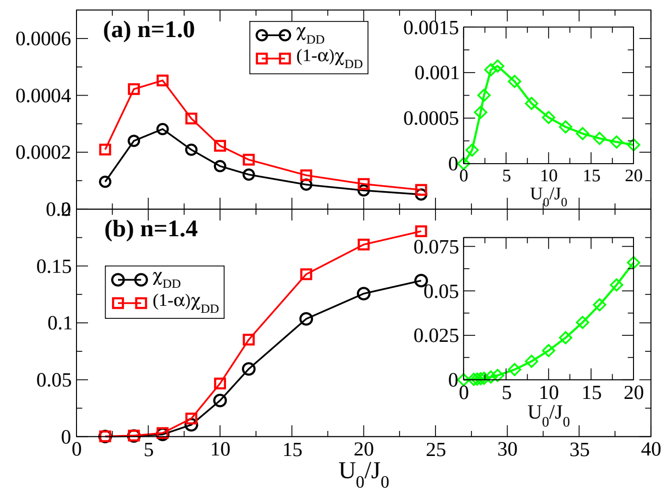

FIG. 1: (Color online). Top panel (a) shows data for half filling, and panel (b) for a filling of $n = 1.4$, for a two-dimensional 4×4 Hubbard lattice. Red curves (squares) show the quantity $(1-\alpha)\chi_{\mathrm{DD}}$, that appears in the linear response of the double occupancy, evaluated at zero Matsubara frequency as a function of U_0/J_0. Neglecting the modulation of the Hubbard interaction amounts to setting $\alpha = 0$, yielding a smaller result (black curve, circles). For comparison, the green diamonds in the insert in both (a) and (b) are exact results for $(1-\alpha)\chi_{\mathrm{DD}}$ for a two-site Hubbard model. α is determined by assuming $a_s/\lambda = 0.0119$, where $a_s = 240a_0$ (a_0 is Bohr radius) and $\lambda = 1,064$ nm (following Ref. [2]), thus α can be found as a single-valued function of U_0/J_0.

To illustrate the importance of incorporating the modulation of the interaction parameter U, in Fig. 1 we show the dependence with U_0/J_0 of the double-occupancy response function $\chi_{\mathrm{DD}}(i\nu_n = 0)$ (black curves), for $n = \langle n_{i\uparrow} + n_{i\downarrow}\rangle = 1.0$ and $n = 1.4$ along with this quantity multiplied by $(1-\alpha)$ (red curve). Therefore, the black curves is the result from modulating δJ only, while the red curve also includes the effect of modulating δU. The difference between the curves illustrates that δU should not be neglected. We observe from Fig. 1 that at half-filling (n=1), the double occupancy response is largest in the intermediate interaction region and decreases with increasing U_0/J_0. This is in striking contrast to the behavior at $n = 1.4$, in which the double occupancy response is small at weak coupling and saturates at large

U_0/J_0. To confirm our numerical calculation, we analytically solved the case of a two-site Hubbard model and found qualitatively similar behavior. (See green curves in Fig. 1.)

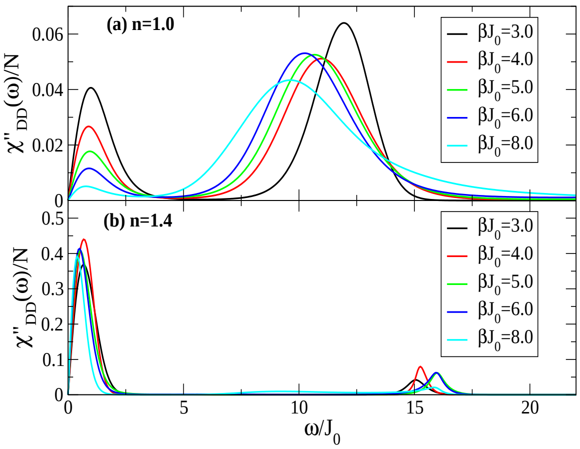

FIG. 2: (Color online). The imaginary component of the double-occupancy susceptibility $\chi''_{\rm DD}(\omega)/N$ for $U_0/J_0 = 10.0$, a 4×4 square lattice, and various values of inverse temperature ($\beta = 1/T$). Panel (a) shows half-filling $n = 1.0$ results, and panel (b) a filling of $n = 1.4$. $N = 16$ is the system size.

We now turn to the full frequency dependent dynamical susceptibility, which determines the response to the dynamical modulation, showing its evolution as a function of temperature (expressed in terms of $\beta J_0 = J_0/k_{\rm B}T$) in Fig. 2. Panel (a) displays results at half-filling, where Mott-insulating physics dominates. At this filling the low frequency response is strongly suppressed for temperatures approaching zero (so that this quasi-peak represents thermally-excited states, not coherent excitations), with the predominant response occurring at frequencies close to U_0. This energy scale, corresponding to the Mott gap, is consistent with recent experimental results [2] which find a strong response in the double occupancy when $\omega \sim U_0$. The presence of the Mott gap also accounts for the much smaller values of χ'' in the top panels of Figs. 1 and 2. Panel (b) shows a filling $n = 1.4$, where an $\omega = 0$ peak remains robust for $T \to 0$. We attribute this peak to the presence of gapless excitations reflecting Fermi liquid behavior in this region. The peak at high ω represents coherent excitations at the band-gap scale which should be the distance between the lower and upper Hubbard bands.

In Fig. 3, we show the interaction dependence of $\chi''_{\rm DD}(\omega)$. Panel (a) displays the half-filled case where the peaks are centered at U_0. In panel (b), filling $n = 1.4$, we include the case of a larger lattice size (6×6) to show that finite size effects are small. These results further verify the important role of filling in the response to dynamical modulation. Our findings can be qualitatively reproduced by neglecting vertex corrections in $\chi_{\rm KK}$ and expressing the single particle Green's function in the Hubbard-I approximation. The latter corresponds to using a approximate self-energy of the form

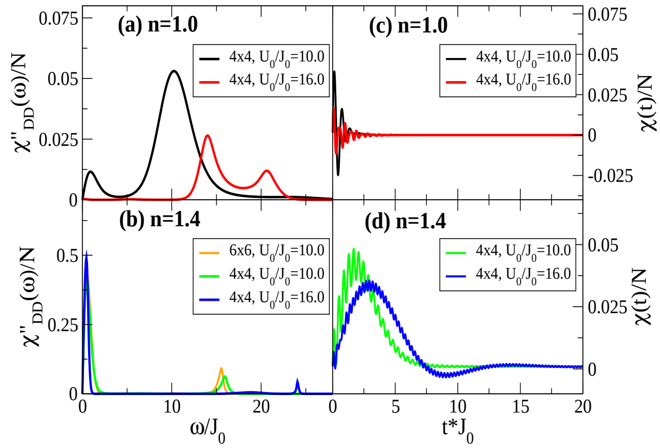

FIG. 3: (Color online). Left column: The imaginary part of the double-occupancy susceptibility $\chi''_{\rm DD}(\omega)/N$ for $U_0/J_0 = 10$ and 16. Panel (a) shows half-filling $n = 1.0$ results for a 4×4 lattice, $U_0/J_0 = 10.0$ (black solid curve) and $U_0/J_0 = 16.0$ (red solid curve). Panel (b) shows results for a filling $n = 1.4$ and for $U_0/J_0 = 10.0$, 6×6 square lattice (orange curve), $U_0/J_0 = 10.0$, 4×4 (green curve), and $U_0/J_0 = 16.0$, 4×4 (blue curve). Right column: The real-time double-occupancy response function $\chi_{\rm DD}(t)$ for a 4×4 square lattice at half filling (panel (c)) for $U_0/J_0 = 10.0$ (black solid curve) and $U_0/J_0 = 16.0$ (red solid); and for $n = 1.4$ (panel (d)) with $U_0/J_0 = 10.0$ (green curve) and $U_0/J_0 = 16.0$ (blue curve). All results are at a temperature $T/J_0 = 2/3$.

$$\Sigma_\sigma(\omega) \sim \frac{U_0^2\, n_{\bar\sigma}(1-n_{\bar\sigma})}{\omega + i\delta}. \qquad (6)$$

We find that $\chi''_{\rm KK}(\omega)$ (and hence $\chi''_{\rm DD}(\omega)$) possess poles at $\omega \sim 0, \pm\sqrt{(\epsilon_{\mathbf k})^2 + 4U_0^2\, n_\sigma(1-n_\sigma)}$, where $\epsilon_{\mathbf k}$ is the energy of a non-interacting quasiparticle with momentum $\mathbf{k}$. In the low energy region, there are quasi-elastic peaks at approximately $\omega \sim 0$. Note that the peak vanishes at $\omega = 0$ because the imaginary part of the real frequency susceptibility is an odd function $\chi''_{\rm KK}(-\omega) = -\chi''_{\rm KK}(\omega)$. In the high energy region, the peaks are located at roughly $\omega \sim U_0 + \frac{\epsilon_{\mathbf k}^2}{2U_0}$. Therefore, at half-filling, the peaks are at $\omega = U_0$ but they sit at higher frequencies away from half filling.

We now turn to the question of how the features in $\chi_{\rm DD}(\omega)$ would be reflected in a experimental measurement of the double occupancy, by inserting our results for $\chi_{\rm DD}(t)$ into Eq. (4). For this task, we need to obtain the real part of $\chi_{\rm DD}(\omega)$ via Kramers-Kronig; upon Fourier transforming we find the real-time dynamical response functions for the double occupancy to be strikingly different at half filling and away from half filling, as

seen in panels (c) and (d) of Fig. 3. We see that filling $n = 1$ shows a response function that is tightly peaked at $t \to 0$, characterized by a single frequency scale $\omega \sim U_0$, while at $n = 1.4$ we see a broad behavior dominated by the two distinct frequencies associated with $\omega \sim 0$ and $\omega \sim U_0 + \frac{\epsilon_{\mathbf{k}}^2}{2U_0}$.

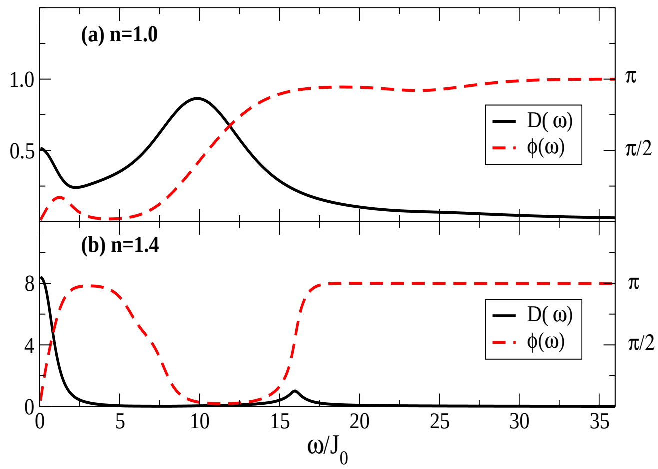

FIG. 4: (Color online). The frequency dependence of the double occupancy linear response for a 4×4 lattice, interaction strength $U_0/J_0 = 10.0$, and temperature $T/J_0 = 2/3$. Panel (a) shows half-filling results; panel (b), $n = 1.4$. Solid (black) curves shows the amplitude $D(\omega)$ while the dashed (red) curves display the phase shift $\phi(\omega)$ induced by the dynamical modulation.

As in standard linear response theory, the real and imaginary parts of $\chi_{\rm DD}(\omega)$ correspond to the in-phase and out of phase parts of the response, respectively. Thus, to linear order, an oscillatory driving of the optical lattice potential yields an oscillatory response at the same frequency, but with a phase lag characterized by the ratio of $\tan\phi(\omega) = \chi''_{\rm DD}(\omega)/\chi'_{\rm DD}(\omega)$. This response has recently been observed directly [12]. We can then write the time-dependent double occupancy as

$$D(t) = D(0) + D(\omega)\sin[\omega t - \phi(\omega)], \qquad (7)$$

where $D(\omega) = U_0/J_0(\alpha - 1)\delta J|\chi_{\rm DD}(\omega)|$. We plot $D(\omega)$ and $\phi(\omega)$ in Fig. 4 for the case of $U_0/J_0 = 10$. We first note that, at low frequency $\omega \to 0$, Eq. (7) implies the time dependence of $D(t)$ to be precisely π out of phase with $\delta V(t)$. Therefore, an adiabatic increase of the optical lattice amplitude leads to a corresponding *suppression* of the double occupancy. At higher ω these plots show how the time-dependent linear response of the double occupancy probes the underlying fermion correlations. As we expected, the half filled case shows the strongest response when the driving frequency $\omega \sim U$, and with a phase that is shifted, by $\phi \approx \pi/2$, relative to the imposed modulation. At $\langle n \rangle = 1.4$, however, the predominant response is for $\omega = 0$, with phase shift $\phi \approx 0$.

In conclusion, we have investigated the dynamical properties of fermions in an optical lattice, realized by the Hubbard model subject to a periodic optical lattice modulation. We show that the modulation of the onsite interaction cannot be neglected and that, even at the level of linear response, the dynamical double occupancy provides a sensitive probe of fermion correlations. Recent cold-atom experiments [12] studying the dynamical modulation of the optical lattice find a linear in time contribution to the double occupancy, known to emerge at quadratic order in the modulation parameter δV [4]. Thus, we expect that our linear-response results apply at smaller $\delta V/V_0$, or after subtracting off this t-linear contribution to focus on the oscillatory component. A future extension of our work will analyze the linear and quadratic-order contributions in detail. In addition, the effects of inhomogeneity due to trapping effects is an issue for future calculations.

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